Bound electron states in the monolayer graphene with the short-range impurities

Natalie E. Firsova
Institute for Problems of Mechanical Engineering, the Russian Academy of Sciences, St. Petersburg 199178, Russia

Sergey A. Ktitorov
A.F. Ioffe Physical-Technical Institute, the Russian Academy of Sciences, St. Petersburg, Russia

Philip A. Pogorelov
St. Petersburg State University, Pervogo Maya str. 100, Petrodvoretz, St. Petersburg 198504, Russia

Bound electron states in impure graphene are considered. Short-range perturbations for defect and impurities of the types "local chemical potential" and "local gap" are taken into account.

I. INTRODUCTION

The Dirac equation is a fundamental base of the relativistic field theory. However, it is an important model in the non-relativistic solid state theory as well. Superconductors with $d-$pairing [1], the Cohen-Blount two-band model of narrow-gap semiconductors [2], [3], electronic spectrum of the carbon tubes form an incomplete list of the non-relativistic applications of this equation. During the last two years extremely much attention was payed to the problem of the electronic spectrum of graphene (see for the review [4]). Two-dimensional structure of it and a presence of the cone points in the electronic spectrum make actual a comprehensive study of the external fields effect on the spectrum and other characteristics of the electronic states described by the Dirac equation in the 2+1 space-time. We consider in this work the bound states of the 2+1 Dirac equation due to the short-range perturbation. Particular attention to this case stems from the effectiveness of short-range scatterers in contrast to the long-range ones: an effect of the latter is suppressed by the Klein paradox [5]. Our work takes into account the obvious fact that the Kohn-Luttinger matrix elements of the short-range perturbation calculated on the upper and lower band wave functions are not equal in a general case. This means that in the perturbed Dirac equation not only the potential but the mass perturbation can be present.

II. PERTURBED DIRAC EQUATION IN (2+1)-SPACE-TIME

The Dirac equation describing electronic states in graphene reads [4]

$$\left(-is\hbar\sum_{\mu=1}^{2}\sigma_\mu\partial_\mu-\sigma_3\left(m+\delta m\right)s^2\right)\psi=\left(E-V\right)\psi, \tag{1}$$

where s is the limiting velocity of the band electrons, σ_μ are the Pauli matrices, $2ms^2=E_g$ is the electronic spectrum gap, $\psi\left(\mathbf{r}\right)$ is the two-component spinor. The spinor structure takes into account the two-band nature. $\delta m\left(\mathbf{r}\right)$ and $V(\mathbf{r})$ are the local perturbations of the mass (gap) and the chemical potential. A local mass perturbation can be induced by defects in the graphene film or in the substrate [6]. We consider here the delta function model of the perturbation:

$$\delta m\left(\mathbf{r}\right)=-b\delta(r-r_0),\ V(\mathbf{r})=-a\delta(r-r_0), \tag{2}$$

where r and r_0 are respectively the polar coordinate radius and the perturbation radius. Such short-range perturbation (and the equivalent form $diag(V_1,V_2)\delta(r-r_0)$ with $-V_1=\frac{a+b}{2},-V_2=\frac{a-b}{2}$) was used in the (3+1)-Dirac problem for narrow-gap and zero-gap semiconductors in [3]. The two-dimensional Dirac problem with the scalar short-range perturbation (2) (but without the mass perturbation) was considered in [7]. The obtained there characteristic equation for the discrete spectrum energy contains one mistake. We correct it here and take account of the mass perturbation $\delta m\left(\mathbf{r}\right)$.

Let us present the two-component spinor in the form

$$\psi_j(\mathbf{r},t)=\frac{\exp\left(-iEt\right)}{\sqrt{r}}\begin{pmatrix}f_j\left(r\right)\exp\left[i\left(j-1/2\right)\phi\right]\\ g_j\left(r\right)\exp\left[i\left(j+1/2\right)\phi\right]\end{pmatrix}, \tag{3}$$

where j is the pseudospin quantum number; $j = \pm 1/2, \pm 3/2, \ldots$. In the opposite to the relativistic theory, this quantum number has nothing to do with the real spin and indicates the degeneracy in the biconic Dirac point. The upper $f_j(r)$ and $g_j(r)$ components of the spinor satisfy the equations

$$\frac{dg_j}{dr} + \frac{j}{r} g_j - (E - m) f_j = (a + b)\, \delta(r - r_0) f_j, \tag{4}$$

$$-\frac{df_j}{dr} + \frac{j}{r} f_j - (E + m) g_j = (a - b)\, \delta(r - r_0) g_j. \tag{5}$$

These equations have a symmetry:

$$f_j \leftrightarrow g_j,\ E \to -E,\ j \to -j \tag{6}$$

Let us introduce the function $\varphi_j(r) \equiv f_j/g_i$. It satisfies the equation:

$$\frac{1}{(a + b)\varphi_j^2 + (a - b)} \left[\frac{d\varphi_j}{dr} - \frac{2j}{r} \varphi_j - E\left(\varphi_j^2 + 1\right) \right] + \delta(r - r_0) = 0 \tag{7}$$

Integrating in the vicinity of $r = r_0$

$$\lim_{\epsilon \to 0} \int_{\varphi_j(r_0 - \epsilon)}^{\varphi_j(r_0 + \epsilon)} \frac{d\varphi_j}{(a + b)\varphi_j^2 + (a - b)} = -1, \tag{8}$$

we obtain the matching condition

$$\arctan\left(\varphi_j^- \sqrt{\frac{a + b}{a - b}}\right) - \arctan\left(\varphi_j^+ \sqrt{\frac{a + b}{a - b}}\right) = \sqrt{a^2 - b^2}, \tag{9}$$

where $\varphi_j^- \equiv \varphi_j(r_0 - \epsilon), \varphi_j^+ \equiv \varphi_j(r_0 + \epsilon), a^2 > b^2$. The upper and lower component matching condition resulting from (9) reads

$$\begin{pmatrix} f_j^+ \\ g_j^+ \end{pmatrix} = \hat{A} \begin{pmatrix} f_j^- \\ g_j^- \end{pmatrix}, \tag{10}$$

where the matrix $\hat{A}$

$$\begin{pmatrix} \cos\sqrt{a^2 - b^2}, & -\sqrt{\frac{a-b}{a+b}} \sin\sqrt{a^2 - b^2} \\ \sqrt{\frac{a-b}{a+b}} \sin\sqrt{a^2 - b^2}, & \cos\sqrt{a^2 - b^2} \end{pmatrix} \tag{11}$$

is orthogonal for $b = 0$. It transmutes into the matrix

$$\begin{pmatrix} \cosh\sqrt{b^2 - a^2}, & -\sqrt{\frac{b-a}{b+a}} \sinh\sqrt{b^2 - a^2} \\ \sqrt{\frac{b-a}{b+a}} \sinh\sqrt{b^2 - a^2}, & \cosh\sqrt{b^2 - a^2} \end{pmatrix}, \tag{12}$$

when $a^2 - b^2 < 0$.

The general solution can be found solving the second-order equation obtained by excluding one of the spinor components from the equation set (4), (5) in the domains $0 < r < r_0$ and $r > r_0$:

$$\frac{d^2 f_j}{dr^2} + \left[E^2 - m^2 - \frac{j(j - 1)}{r^2} \right] f_j = 0. \tag{13}$$

This equation is related to the Bessel one. Its general solution reads

$$f_j = C_1 \sqrt{r} I_{j-1/2}(\kappa r) + C_2 \sqrt{r} K_{j-1/2}(\kappa r), \tag{14}$$

where $\kappa^2 = m^2 - E^2$, $I_\nu(z)$ and $K_\nu(z)$ are the modified Bessel functions. The constant $C_2 = 0$ in the domain $0 < r < r_0$, while $C_1 = 0$ in the domain $r > r_0$. Expressing the g_j-component using (5), we can write

$$\varphi_j^- = \sqrt{\frac{m+E}{m-E}} \frac{I_{j-1/2}(\kappa r_0)}{I_{j+1/2}(\kappa r_0)}, \tag{15}$$

$$\varphi_j^+ = \sqrt{\frac{m+E}{m-E}} \frac{K_{j-1/2}(\kappa r)}{K_{j+1/2}(\kappa r)}. \tag{16}$$

Applying the matching condition (9) to the expressions (16), (15) we obtain the characteristic equation for the bound state energy levels:

$$\kappa \left[\frac{K_{j-1/2}(\kappa r_0)}{K_{j+1/2}(\kappa r_0)} - \frac{I_{j-1/2}(\kappa r_0)}{I_{j+1/2}(\kappa r_0)} \right] =$$

$$- \frac{\tan\left(\sqrt{a^2-b^2}\right)}{\sqrt{a^2-b^2}} \left[(m-E)(a-b) + (a+b)(m+E) \frac{I_{j-1/2}(\kappa r_0)}{I_{j+1/2}(\kappa r_0)} \frac{K_{j-1/2}(\kappa r_0)}{K_{j+1/2}(\kappa r_0)} \right] \tag{17}$$

where $a^2 - b^2 > 0$. This equation turns to the characteristic equation obtained in [7], for $b = 0$ apart from the mistakenly omitted terms in the right hand side of (17). In the opposite case of $a^2 - b^2 < 0$ we have

$$\kappa \left[\frac{K_{j-1/2}(\kappa r_0)}{K_{j+1/2}(\kappa r_0)} - \frac{I_{j-1/2}(\kappa r_0)}{I_{j+1/2}(\kappa r_0)} \right] =$$

$$- \frac{\tanh\left(\sqrt{b^2-a^2}\right)}{\sqrt{b^2-a^2}} \left[-(m-E)(b-a) + (b+a)(m+E) \frac{I_{j-1/2}(\kappa r_0)}{I_{j+1/2}(\kappa r_0)} \frac{K_{j-1/2}(\kappa r_0)}{K_{j+1/2}(\kappa r_0)} \right] \tag{18}$$

We write these equations in another form making the symmetry (6) manifest:

$$\kappa \left[I_{j-1/2}(\kappa r_0) K_{j+1/2}(\kappa r_0) - K_{j-1/2}(\kappa r_0) I_{j+1/2}(\kappa r_0) \right] =$$

$$\frac{\tan\left(\sqrt{a^2-b^2}\right)}{\sqrt{a^2-b^2}} \left[(m-E)(a-b) I_{j+1/2}(\kappa r_0) K_{j+1/2}(\kappa r_0) + (a+b)(m+E) I_{j-1/2}(\kappa r_0) K_{j-1/2}(\kappa r_0) \right], \tag{19}$$

$$\kappa \left[I_{j-1/2}(\kappa r_0) K_{j+1/2}(\kappa r_0) - K_{j-1/2}(\kappa r_0) I_{j+1/2}(\kappa r_0) \right] =$$

$$\frac{\tanh\left(\sqrt{b^2-a^2}\right)}{\sqrt{b^2-a^2}} \left[-(m-E)(b-a) I_{j+1/2}(\kappa r_0) K_{j+1/2}(\kappa r_0) + (b+a)(m+E) I_{j-1/2}(\kappa r_0) K_{j-1/2}(\kappa r_0) \right] \tag{20}$$

III. ANALYSIS OF THE CHARACTERISTIC EQUATION AND NUMERICAL RESULTS

Making use of the Bessel functions limiting forms for small arguments [8]

$$I_\nu(z) \sim (z/2)^\nu \frac{1}{\Gamma(\nu+1)}, \; K_0(z) \sim -\ln z, \; K_\nu(z) \sim \frac{1}{2}\Gamma(\nu)(z/2)^{-\nu},$$

we can obtain a simple relation describing the asymptotic behaviour of the energy level, where the perturbation power approaches zero:

$$E = m \left[1 - \frac{r_c^2}{2r_0^2} \exp\left(-\frac{r_c}{r_0(a+b)} \right) \right], \tag{21}$$

where $r_c = m^{-1}$ (in units with $\hbar = s = 1$), $a + b > 0$. This result conforms the well known general property of the two-dimensional quantum systems: a threshold for creation of the bound state is absent; the point $a + b = 0$ is the essentially singular point of the function $E = E(a + b)$. One can see that the function $E(a)$ approaches the point $E = -m$ at some large enough value of $a > 0$. . Making use of the Bessel function asymptotic behaviour [8],

$$I_\nu(z) \sim (2\pi z)^{-1/2} \exp z,\ K_\nu(z) \sim \left(\frac{\pi}{2z}\right)^{1/2} \exp(-z),$$

and the equation 18, we can see that the function $E(b)$ approaches the point $E = 0$ when $\frac{r_0}{r_c}$ is large enough and $b \to \infty$.

In the Fig. 1 the electron bound state energy is presented as a function of the potential amplitude for the angular momentum quantum number $j = 1/2$, $\frac{r_0}{r_c} = 1$ and $b = 0$. Inspecting this plot one can see that our analytic solution (21) perfectly approximates approaching of the bound state energy value the upper band bottom, when b approaches zero.

In the Fig. 2 the bound state energy is presented as a function of the mass perturbation amplitude b for $a = 0$, $\frac{r_0}{r_c} = 1$, $j = 1/2$.

In the Fig. 3 the electron bound state energy is presented as a function of the potential amplitude for the angular momentum quantum number $j = 1/2$, $\frac{r_0}{r_c} = 1$, and $b = -1$. We see that the energy dependence on a is non-monotonic function, but approaching the upper band bottom takes place similarly to the case of $b = 0$.

IV. CONCLUSION

In conclusion, we considered the bound electron states for the two-dimensional Dirac equation with the short-range perturbation. The short-range perturbation is approximated by the delta function $\delta(r - r_0)$ with different amplitudes in the upper and lower bands. We found the characteristic equation for the discrete energy levels. Energy levels behaviour in dependence on the perturbation amplitudes was investigated both analytically and numerically. The obtained results can be useful for understanding of the graphene electron properties.

[1] D.J. Scalapino, Phys. Rep. **250**, 329 (1995).
[2] L.V. Keldysh, JETP **45**, 365 (1963).
[3] S.A. Ktitorov, V.I. Tamarchenko, Soviet Physics (Solid State) **19**, 2070 (1977).
[4] A.H. Castro Neto, F. Guinea, et al, arXiv: 0709.1163 (2008) (accepted to Rev. Mod. Phys).
[5] C.W.J. Beenakker, Rev. Mod. Phys., **80**, 1337 (2008).
[6] Aurelien Lherbier, X. Blaze, et al, Phys. Rev. Letters, **101**, 036808-1 (2008).
[7] Shi-Hai Dong, Zhong-Qi Ma, Phys. Lett. A **15**, 171 (2002).
[8] M. Abramowitz, I.A. Stegun, *Handboock of Mathematical Functions with Formulas, Graphs, and Mathematical Tables,* National Bureau of Standards, Washington DC, 1964.

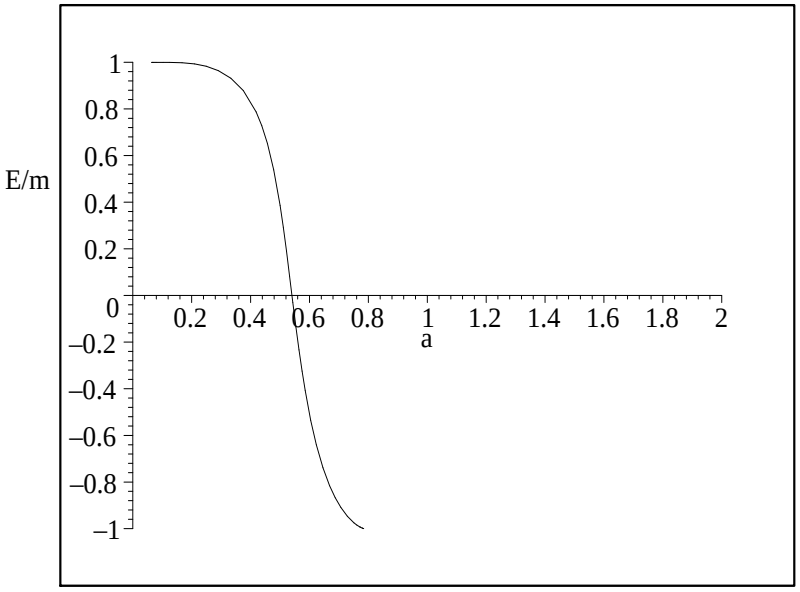

FIG. 1: Reduced lower electron bound state energy E/m dependence on the short-range potential amplitude a at b=0.

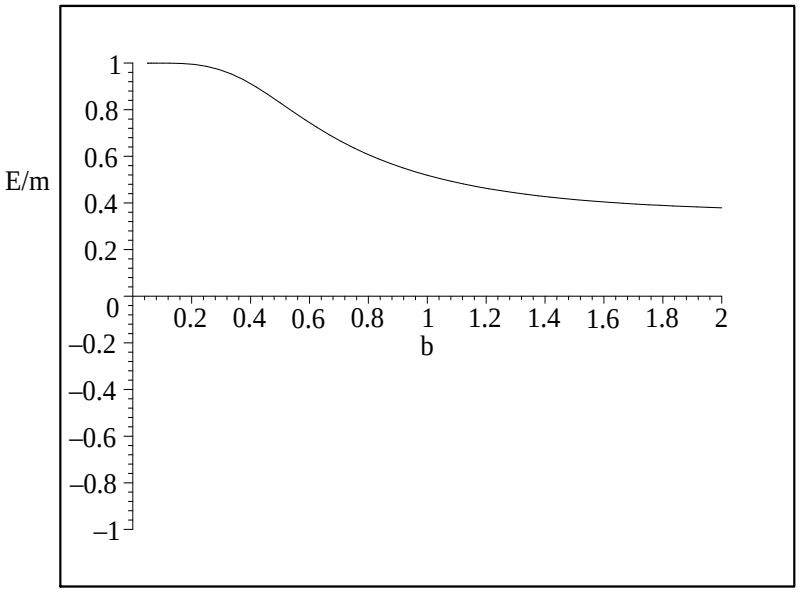

FIG. 2: Reduced lower electron bound state energy E/m dependence on the mass perturbation amplitude b at a=0.

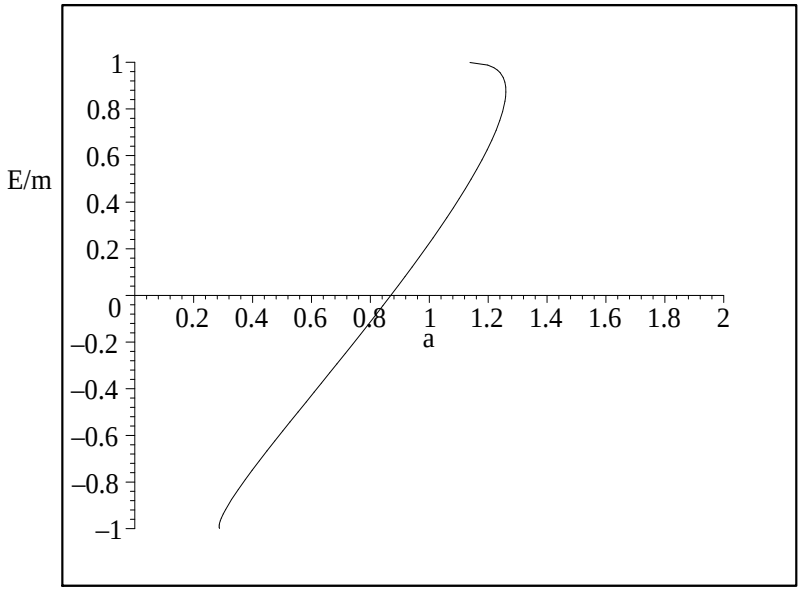

FIG. 3: Reduced lower electron bound state energy E/m dependence on the short-range potential amplitude a at b=-1.